An individual-based modeling approach for cellulose degradation by microbial biofilms

Ariane Bize[1]*, Fabien Campillo[2], Chloé Deygout[2], Claude Lobry[2], Marc Joannides[2-3]

1 Irstea, UR HBAN, F-92761, Antony, France. **2 INRIA, MODEMIC** project-team / **INRA, UMR MISTEA**, Montpellier, France
3 Université Montpellier 2/I3M, Montpellier, France.

***ariane.bize@irstea.fr**

Context. Cellulose is the most abundant renewable biopolymer on Earth and it is recalcitrant to degradation. Optimizing its anaerobic digestion is a key-issue in the field of bioenergy. During this bioprocess, cellulolytic bacteria adhere to – and form a thin biofilm around – cellulose particles. Modeling approaches can help understanding these complex processes (reviewed in Lynd et al., 2002, Lübken et al., 2010).

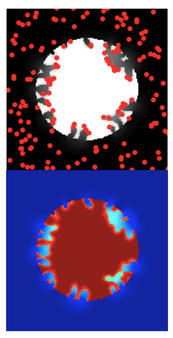
Main conclusions. The individual-based model (IBM) developed here accounts for biofilm formation with minimal hypotheses: soluble substrate diffusion combined with bacterial chemotaxis-like movement in the liquid phase, lack of bacterial movement in the solid phase. The IBM results are qualitatively different from the main macroscopic degradation models previously used for cellulose degradation. It suggests that random and discrete processes could significantly impact the cellulose degradation dynamics by their effect on the spatial structuration of the colonized cellulose particles.

IBM description: hydrolysis of one cellulose fiber slice by individual bacterial cells

Model state variables

For each bacterial cell
- continuous position (*x, y*)
- carbon mass *m*

For cellulose and its hydrolysis products
- surfacic carbon density *C*
  (carbon is the bacterial growth substrate)



An original representation of the cellulose and its hydrolysis products

Continuous representation of carbon in its insoluble (cellulose) or soluble (cellodextrines) state by *C(t,x)*

C(t,x)	Physical phase	Carbon state	Carbon diffusion	Bacterial movement
$> C_{diff}$	solid	polymerized	no	no
$\leq C_{diff}$	liquid	soluble	yes	yes

→ Non-explicit degree of polymerization of the glucose molecules

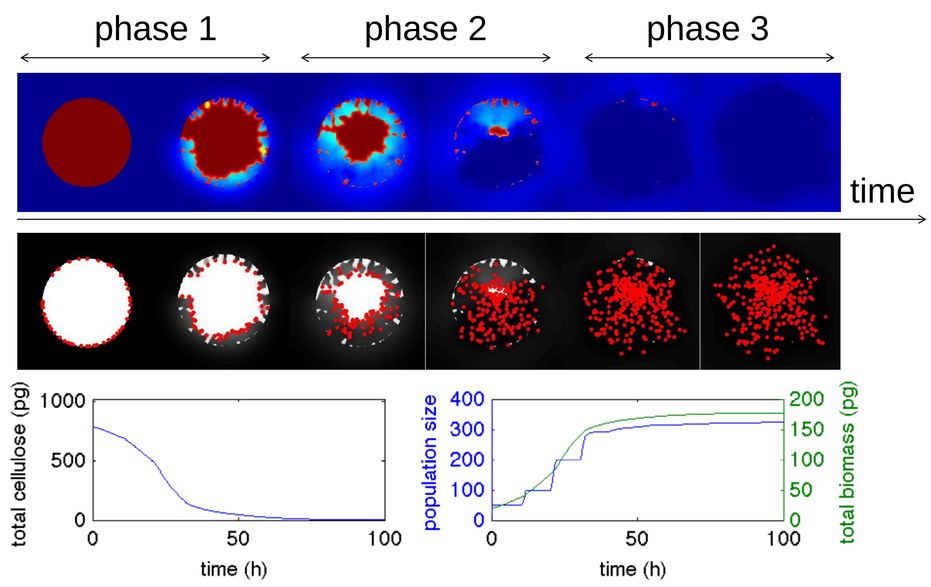
Model dynamics

Actions at each time step	Main features
soluble carbon diffusion	Fick's law
bacterial movement	sum of a random component and of a component proportional to the local carbon gradient density
bacterial substrate uptake	each cell feeds on the carbon available in its neighborhood and in proportion to its mass
bacterial growth	substrate -to-biomass carbon conversion with a yield coefficient
bacterial division	when a critical mass is reached, cell division generates 2 cells with identical positions and similar masses

IBM result: a sudden degradation acceleration

3 temporal phases are schematically distinguished

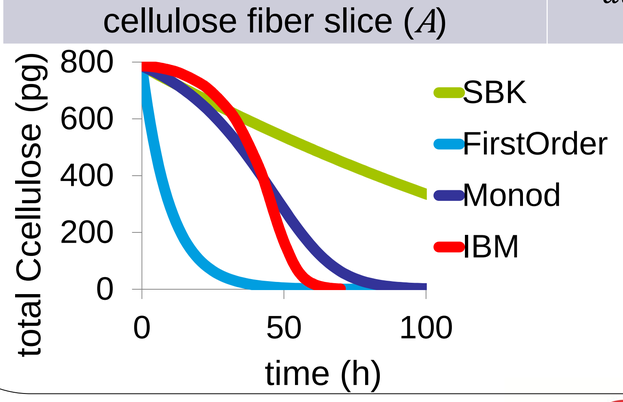
- **phase 1: slow degradation** due to the limited colonized cellulose surface
- **phase 2: pronounced acceleration** of the degradation due to the important colonized surface generated by bacterial movement and feeding, shaping an irregular cellulose structure
- **phase 3: pronounced deceleration** of the degradation due to substrate exhaustion



Representative simulation results. Upper pannel: carbon density. Middle pannel: bacterial cells. Lower pannel: aggregated values for cellulosic carbon (left), biomass carbon and bacterial population size (right).

Comparison with classical cellulose degradation models: qualitatively distinct kinetics

Reference models (reviewed in Lübken et al., 2010)	Equations C, cellulose B, biomass	Parameter values
First order kinetics	$\frac{dC}{dt} = -k.C$	$k = 0.1$
Monod model	$\frac{dC}{dt} = -\frac{u.C.B}{K+C}$	$u \approx 0.35$ $K \approx 523$
Surface based kinetics (SBK) considering the latteral area of the cellulose fiber slice (A)	$\frac{dC}{dt} = -k.A$	$k \approx 0.09$



Identical initial population sizes for all the models. Non-adjusted parameters, physical values are used. For the IBM, the average of 500 Monte Carlo simulations is shown.

References.

Lynd et al. (2002) Microbiology and Molecular Biology Reviews. 66:506–577

Lübken et al. (2010). Applied Microbiology and Biotechnoly. 85:1643–1652.

ANR SYSCOMM / DISCO project

www.irstea.fr